

IMSc/04/01/01<sup>†</sup>

# QUANTUM MECHANICS OF DIRAC PARTICLE BEAM OPTICS: SINGLE-PARTICLE THEORY

R. JAGANATHAN

*The Institute of Mathematical Sciences**4th Cross Road, Central Institutes of Technology Campus**Tharamani, Chennai - 600113, Tamilnadu, INDIA**E-mail: [jagan@imsc.ernet.in](mailto:jagan@imsc.ernet.in) - URL: <http://www.imsc.ernet.in/~jagan>*

It has been found that quantum corrections can substantially affect the classical results of tracking for trajectories close to the separatrix. Hence the development of a basic formalism for obtaining the quantum maps for any particle beam optical system is called for. To this end, it is observed that several aspects of quantum maps for the beam optics of spin- $\frac{1}{2}$  particles can be studied, at the level of single particle dynamics, using the proper formalism based on the Dirac equation.

## 1 Introduction

The theory of particle beam optics, currently used in the design and operation of various beam devices, from electron microscopes to accelerators, is largely based on classical mechanics and classical electrodynamics. Such a treatment has indeed been very successful in practice. Of course, whenever it is essential, quantum mechanics is used in accelerator physics to understand those quantum effects which are prominent perturbations to the leading classical beam dynamics [1]. The well-known examples are quantum excitations induced by synchrotron radiation in storage rings, the Sokolov-Ternov effect of spin polarization induced by synchrotron radiation, etc. Recently, attention has been drawn by Hill [2] to the limits placed by quantum mechanics on achievable beam spot sizes in particle accelerators, and the need for the formulation of quantum beam optics relevant to such issues [3]. In the context of electron microscopy scalar wave mechanics is the main tool to understand the image formation and its characteristics, and the spin aspects are not generally essential [4].

In the context of accelerator physics it should be certainly desirable to have a unified framework based entirely on quantum mechanics to treat the orbital, spin,

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<sup>†</sup>To appear in the Proceedings of the 18th Advanced ICFA Beam Dynamics Workshop on Quantum Aspects of Beam Physics, October 15-20, 2000, Capri, Italy, Ed. Pisin Chen (World Scientific, Singapore)

radiation, and every aspect of beam dynamics, since the constituents of the beams concerned are quantum particles. First, this should help us understand better the classical theory of beam dynamics. Secondly, there is already an indication that this is necessary too: it has been found [5] that quantum corrections can substantially affect the classical results of tracking for trajectories close to the separatrix, leading to the suggestion that quantum maps can be useful in finding quickly the boundaries of nonlinear resonances. Thus, a systematic formalism for obtaining the relevant quantum maps is required. This problem is addressed here for the case of spin- $\frac{1}{2}$  particle beams, at the level of single particle dynamics as the first step towards a more comprehensive theory.

## 2 Quantization of the classical particle beam optics

If the spin is ignored, one may consider obtaining the relevant quantum maps for any beam optical system by quantizing the corresponding classical treatment directly. The best way to do this is to use the Lie approach to classical beam dynamics, thoroughly developed by Dragt *et al.*, [6] particularly in the context of accelerator physics. Ignoring the effect of spin on the orbital motion, the spin motion has also been treated classically, independent of the orbital motion, using Lie methods [7].

Let the single particle optical Hamiltonian corresponding to a classical beam optical system be  $\mathcal{H}(\underline{r}_\perp, \underline{p}_\perp; z)$ , where  $z$  is the coordinate along the optic axis of the system, and  $\underline{r}_\perp = (x, y)$  and  $\underline{p}_\perp = (p_x, p_y)$  represent the coordinates and conjugate momenta, respectively, in the transverse  $(x, y)$ -plane. We shall assume the beam to be moving in the positive  $z$ -direction. Then for any observable of the system,  $\mathcal{O}(\underline{r}_\perp, \underline{p}_\perp)$ , not explicitly dependent on  $z$ , the  $z$ -evolution equation, or the beam optical equation of motion, is

$$\frac{d\mathcal{O}}{dz} =: -\mathcal{H} : \mathcal{O}, \quad (1)$$

where the Lie operator  $: f :$  associated with any function of the transverse phase-space variables,  $f(\underline{r}_\perp, \underline{p}_\perp)$ , is defined through the Poisson bracket,

$$: f : g = \{f, g\} = \left( \frac{\partial f}{\partial x} \frac{\partial g}{\partial p_x} - \frac{\partial f}{\partial p_x} \frac{\partial g}{\partial x} \right) + \left( \frac{\partial f}{\partial y} \frac{\partial g}{\partial p_y} - \frac{\partial f}{\partial p_y} \frac{\partial g}{\partial y} \right). \quad (2)$$

When the Hamiltonian  $\mathcal{H}$  is  $z$ -independent the solution of Eq. (1) can be written down as

$$\mathcal{O}(z_f) = \exp(\ell : -\mathcal{H} :) \mathcal{O}(z_i)$$

$$\begin{aligned}
&= \mathcal{O}(z_i) + \ell(\colon -\mathcal{H} : \mathcal{O})(z_i) + (\ell^2/2!) (\colon -\mathcal{H} :^2 \mathcal{O})(z_i) \\
&\quad + (\ell^3/3!) (\colon -\mathcal{H} :^3 \mathcal{O})(z_i) + \dots \\
&= \mathcal{O}(z_i) + \ell(\{-\mathcal{H}, \mathcal{O}\})(z_i) + (\ell^2/2!) (\{-\mathcal{H}, \{-\mathcal{H}, \mathcal{O}\}\})(z_i) \\
&\quad + (\ell^3/3!) (\{-\mathcal{H}, \{-\mathcal{H}, \{-\mathcal{H}, \mathcal{O}\}\}\})(z_i) + \dots, \tag{3}
\end{aligned}$$

relating  $\mathcal{O}(z_i)$ , the value of  $\mathcal{O}$  at an initial  $z_i$ , with  $\mathcal{O}(z_f)$ , its value at a final  $z_f$ , where  $z_f > z_i$  and  $\ell = (z_f - z_i)$ . When the Hamiltonian depends on  $z$  we would have

$$\mathcal{O}(z_f) = \left( \wp \left[ \exp \left( \int_{z_i}^{z_f} dz : -\mathcal{H} : \right) \right] \mathcal{O} \right)(z_i) = (\mathcal{M}(z_f, z_i) \mathcal{O})(z_i), \tag{4}$$

where the transfer map,  $\mathcal{M}(z_f, z_i)$ , a Lie transformation, is now an  $z$ -ordered exponential.

To obtain the quantum mechanical formalism for the above system we can follow the canonical quantization rule  $\{ \ , \ } \longrightarrow \frac{1}{i\hbar} [ \ , \ ]$  where  $[ \ , \ ]$  represents the commutator bracket between the corresponding quantum operators. This turns Eq. (1) into the Heisenberg equation of motion

$$\frac{d\hat{\mathcal{O}}}{dz} = \frac{i}{\hbar} [\hat{\mathcal{H}}, \hat{\mathcal{O}}], \tag{5}$$

where the quantum Hamiltonian operator  $\hat{\mathcal{H}}$ , and  $\hat{\mathcal{O}}$  for any observable, are obtained from their respective classical counterparts by the replacement

$$\underline{r}_\perp \longrightarrow \hat{\underline{r}}_\perp = \underline{r}_\perp = (x, y), \quad \underline{p}_\perp \longrightarrow \hat{\underline{p}}_\perp = -i\hbar \underline{\nabla}_\perp = \left( -i\hbar \frac{\partial}{\partial x}, -i\hbar \frac{\partial}{\partial y} \right), \tag{6}$$

followed by a symmetrization to ensure that the quantum operators are hermitian.

From the Heisenberg picture of Eq. (5) let us go to the Schrödinger picture in which a wavefunction  $\psi(\underline{r}_\perp; z)$  is associated with the transverse plane at  $z$ . The  $z$ -evolution of  $|\psi(z)\rangle$  is governed by the beam optical Schrödinger equation

$$i\hbar \frac{\partial}{\partial z} |\psi(z)\rangle = \hat{\mathcal{H}} |\psi(z)\rangle. \tag{7}$$

Since  $|\psi(\underline{r}_\perp; z)|^2$  will represent the probability density in the transverse plane at  $z$  the average of any  $\hat{\mathcal{O}}$  at  $z$  will be

$$\langle \hat{\mathcal{O}} \rangle(z) = \int \int dx dy \psi^*(z) \hat{\mathcal{O}} \psi(z) = \langle \psi(z) | \hat{\mathcal{O}} | \psi(z) \rangle, \tag{8}$$

with  $\psi(\underline{r}_\perp; z)$  normalized as  $\langle \psi(z) | \psi(z) \rangle = 1$ .

The formal solution of Eq. (7) is, with  $|\psi_i\rangle = |\psi(z_i)\rangle$  and  $|\psi_f\rangle = |\psi(z_f)\rangle$ ,

$$|\psi_f\rangle = \hat{U}(z_f, z_i) |\psi_i\rangle = \hat{U}_{fi} |\psi_i\rangle, \quad \hat{U}_{fi} = \wp \left[ \exp \left( -\frac{i}{\hbar} \int_{z_i}^{z_f} dz \hat{\mathcal{H}} \right) \right]. \quad (9)$$

Thus, we get

$$\langle \hat{\mathcal{O}} \rangle_f = \langle \hat{\mathcal{O}} \rangle(z_f) = \langle \psi_f | \hat{\mathcal{O}} | \psi_f \rangle = \langle \psi_i | \hat{U}_{fi}^\dagger \hat{\mathcal{O}} \hat{U}_{fi} | \psi_i \rangle = \langle \hat{U}_{fi}^\dagger \hat{\mathcal{O}} \hat{U}_{fi} \rangle_i. \quad (10)$$

From the correspondence between Eq. (1) and Eq. (5) it follows immediately that

$$\hat{U}_{fi}^\dagger \hat{\mathcal{O}} \hat{U}_{fi} = \left( \wp \left[ \exp \left( \int_{z_i}^{z_f} dz : \frac{i}{\hbar} \hat{\mathcal{H}} : \right) \right] \right) \hat{\mathcal{O}} = \hat{\mathcal{M}}(z_f, z_i) \hat{\mathcal{O}}, \quad (11)$$

with the definition  $: \frac{i}{\hbar} \hat{\mathcal{H}} : \hat{\mathcal{O}} = \frac{i}{\hbar} [\hat{\mathcal{H}}, \hat{\mathcal{O}}]$ . Note that in the classical limit, when  $: \frac{i}{\hbar} \hat{\mathcal{H}} : \hat{\mathcal{O}} \longrightarrow : -\mathcal{H} : \mathcal{O}$ , the quantum Lie transformation  $\hat{\mathcal{M}}(z_f, z_i)$  becomes the classical Lie transformation  $\mathcal{M}(z_f, z_i)$ . This shows that if a system corresponds classically to a map

$$(\underline{r}_{\perp i}, \underline{p}_{\perp i}) \longrightarrow (\underline{r}_{\perp f}, \underline{p}_{\perp f}) = (\underline{R}_{\perp}(\underline{r}_{\perp i}, \underline{p}_{\perp i}), \underline{P}_{\perp}(\underline{r}_{\perp i}, \underline{p}_{\perp i})), \quad (12)$$

then it will correspond to a map of quantum averages as given by

$$\langle \hat{\underline{r}}_{\perp} \rangle_i \longrightarrow \langle \hat{\underline{r}}_{\perp} \rangle_f = \langle \hat{\underline{R}}_{\perp}(\hat{\underline{r}}_{\perp}, \hat{\underline{p}}_{\perp}) \rangle_i, \quad \langle \hat{\underline{p}}_{\perp} \rangle_i \longrightarrow \langle \hat{\underline{p}}_{\perp} \rangle_f = \langle \hat{\underline{P}}_{\perp}(\hat{\underline{r}}_{\perp}, \hat{\underline{p}}_{\perp}) \rangle_i. \quad (13)$$

To see what Eq. (13) implies let us consider, for example, a classical Lie transformation  $\exp \left( : \frac{a}{3} x^3 : \right)$  corresponding to a kick in the  $xz$ -plane by a thin sextupole. This leads to the classical phase-space map

$$x_f = x_i, \quad p_f = p_i + a x_i^2, \quad (14)$$

as follows from Eq. (4). This would correspond to the quantum Lie transformation  $\exp \left( : \frac{a}{3} \hat{x}^3 : \right)$  which leads, as seen from Eq. (13), to the following map for the quantum averages:

$$\langle \hat{x} \rangle_f = \langle \hat{x} \rangle_i, \quad \langle \hat{p} \rangle_f = \langle \hat{p} \rangle_i + a \langle \hat{x}^2 \rangle_i = \langle \hat{p} \rangle_i + a \langle \hat{x} \rangle_i^2 + a \langle (\hat{x} - \langle \hat{x} \rangle)^2 \rangle_i. \quad (15)$$

Now, we can consider the expectation values, such as  $\langle \hat{x} \rangle$  and  $\langle \hat{p} \rangle$ , as corresponding to their classical values *à la* Ehrenfest. Then, as the above simple example shows, generally, the leading quantum effects on the classical beam optics can be expected to be due to the uncertainties in the initial conditions like the term  $a \langle (\hat{x} - \langle \hat{x} \rangle)^2 \rangle_i$  in Eq. (15). As pointed out by Heifets and Yan, [5] such leading quantum corrections involve the Planck constant  $\hbar$  not explicitly but only through the uncertainty principle which controls the minimum limits for the initial conditions. This has been

realized earlier also [8, 9, 10], particularly in the context of electron microscopy [8, 9]. In a detailed study [5] of a simple example it has been found that trajectories close to the separatrix are strongly perturbed in spite of very small initial rms ( $10^{-15}$ ) and small (1500) number of turns.

As is clear from the above, a quantum formalism derived from the classical beam optics can be expected to give all the leading quantum corrections to the classical maps. The question that arises is how to go beyond and obtain the quantum maps more completely starting *ab initio* with the quantum mechanics of the concerned system since such a process should lead to other quantum corrections not derivable simply from the quantization of the classical optical Hamiltonian. Essentially, one should obtain the quantum beam optical Hamiltonian  $\hat{\mathcal{H}}$  of Eq. (7) directly from the original time-dependent Schrödinger equation of the system. Once  $\hat{\mathcal{H}}$  is obtained Lie methods [6, 7] can be used to construct the quantum  $z$ -evolution operator  $\hat{U}_{fi}$  and study the consequent quantum maps. Derivations of  $\hat{\mathcal{H}}$  for the Klein-Gordon and Dirac particle beams will be discussed in the following sections.

A more complete theory, even at the level of optics, must take into account multiparticle effects. To this end, it might be profitable to be guided by the models developed by Fedele *et al.* [11, 12] (thermal wave model - TWM) and Cufaro Petroni *et al.* [13] (stochastic collective dynamical model - SCDM) for treating the beam phenomenologically as a quasiclassical many-body system. Though the details of approach and interpretation are different, both these models suggest phenomenological Schrödinger-like wavefunction descriptions for the collective motion of the beam. In TWM the beam emittance plays the role of  $\hbar$ . In SCDM it is argued that  $\hbar$  is to be replaced by an effective unit of beam emittance given in terms of the Compton wavelength of the beam particle and the number of particles in the beam. It may be noted that Lie algebraic tools can be used to handle any Schrödinger-like equation.

### 3 Using the Klein-Gordon equation ignoring the spin

One may consider getting a theory of quantum maps for spin- $\frac{1}{2}$  particle beam optical system based on the Klein-Gordon equation ignoring the spin. For this, one has to transform the equation

$$\left(i\hbar\frac{\partial}{\partial t} - q\hat{\phi}\right)^2 \Psi(\underline{r}_\perp, z; t) = \left\{c^2 \left[\hat{\pi}_\perp^2 + \left(-i\hbar\frac{\partial}{\partial z} - q\hat{A}_z\right)^2\right] + m^2c^4\right\} \Psi(\underline{r}_\perp, z; t), \quad (16)$$

into the beam optical form in Eq. (7); in Eq.(16)  $q$  is the charge of the particle,  $\hat{\pi}_\perp = (\hat{\pi}_x, \hat{\pi}_y) = (\hat{p}_x - q\hat{A}_x, \hat{p}_y - q\hat{A}_y)$ ,  $\hat{\pi}_\perp^2 = \hat{\pi}_x^2 + \hat{\pi}_y^2$ , and  $\hat{\phi}$  and  $\underline{A} = (A_x, A_y, A_z)$

are, respectively, the scalar and vector potentials of the electric and magnetic fields of the optical system ( $\underline{E} = -\nabla\phi$ ,  $\underline{B} = \nabla \times \underline{A}$ ). In the standard relativistic quantum theory [14], Feshbach-Villars and Foldy-Wouthuysen techniques are used for reducing the Klein-Gordon equation to its nonrelativistic approximation plus the relativistic corrections. Applying analogous techniques in the special case of a quasi-paraxial ( $|\underline{p}_\perp| \ll p_z$ ) monoenergetic beam propagating through a system with time-independent fields one can reduce Eq. (16) to the beam optical form of Eq. (7) with  $\hat{\mathcal{H}}$  containing a leading paraxial part followed by nonparaxial parts [8, 9, 15]. In this case the wavefunction in Eq. (16) can be assumed to be of the form

$$\Psi(\underline{r}_\perp, z; t) = \psi(\underline{r}_\perp; z) \exp \left[ \frac{i}{\hbar} (p_0 z - Et) \right], \quad (17)$$

where  $p_0$  is the design momentum of the beam and  $E = +\sqrt{c^2 p_0^2 + m^2 c^4}$ . Then the resulting time-independent equation for  $\psi(\underline{r}_\perp; z)$  can be regarded as describing the scattering of the beam particle by the system and transformed into an equation of the type in Eq. (7) [8, 9, 15].

For example, for a normal magnetic quadrupole lens with  $\underline{A} = (0, 0, \frac{1}{2}K(x^2 - y^2))$ , where  $K$  is nonzero inside the lens region and zero outside,

$$\hat{\mathcal{H}} \approx \frac{1}{2p_0} (\hat{p}_x^2 + \hat{p}_y^2) - \frac{1}{2}qK(\hat{x}^2 - \hat{y}^2) + \frac{1}{8p_0^3} (\hat{p}_x^2 + \hat{p}_y^2)^2 + \frac{qK\hbar^2}{4p_0^4} (\hat{p}_x^2 - \hat{p}_y^2). \quad (18)$$

It must be noted that while the first three terms of  $\hat{\mathcal{H}}$  in Eq. (18) are exactly the terms derivable by direct quantization of the classical beam optical Hamiltonian the last,  $\hbar$ -dependent, term is a quantum correction not derivable from the classical theory. Though such  $\hbar$ -dependent terms may seem to be too small, particularly for high energy beams, they may become effective when there are large fluctuations in the initial conditions since they essentially modify the coefficients in the classical maps.

## 4 The proper theory using the Dirac equation

For a spin- $\frac{1}{2}$  particle beam the proper theory should be based on the Dirac equation if one wants to treat all the aspects of beam optics including spin evolution and spin-orbit interaction. In such a case the Schrödinger equation to start with is

$$i\hbar \frac{d}{dt} \Psi(\underline{r}_\perp, z; t) = \hat{H} \Psi(\underline{r}_\perp, z; t), \quad (19)$$

where  $\Psi$  is now a 4-component spinor and  $\hat{H}$  is the Dirac Hamiltonian

$$\hat{H} = \beta mc^2 + q\hat{\phi} + c\underline{\alpha}_\perp \cdot \underline{\hat{\pi}}_\perp + c\alpha_z \left( -i\hbar \frac{\partial}{\partial z} - q\hat{A}_z \right) - \mu_a \beta \underline{\Sigma} \cdot \underline{B}, \quad (20)$$

including the Pauli term to take into account the anomalous magnetic moment  $\mu_a$ . In Eq. (20) all the symbols have the usual meanings as in the standard Dirac theory [14]. Considering the special case of a quasiparaxial monoenergetic beam we can take  $\Psi(\underline{r}_\perp, z; t)$  to be of the form in Eq. (17). Then the 4-component  $\psi(\underline{r}_\perp; z)$  satisfies the time-independent Dirac equation

$$\left[ \beta mc^2 + q\hat{\phi} + c\underline{\alpha}_\perp \cdot \hat{\underline{\pi}}_\perp + c\alpha_z \left( -i\hbar \frac{\partial}{\partial z} - q\hat{A}_z \right) - \mu_a \beta \underline{\Sigma} \cdot \underline{B} \right] \psi(\underline{r}_\perp; z) = E\psi(\underline{r}_\perp; z) . \quad (21)$$

describing the scattering of the beam particle by the system.

Actually Eq. (21) has the ideal structure for our purpose since it is already linear in  $\frac{\partial}{\partial z}$ . So one can readily rearrange the terms in it to get the desired form of Eq. (7). However, it is difficult to work directly with such an equation since there are problems associated with the interpretation of the results using the traditional Schrödinger position operator [16]. In the standard theory the Foldy-Wouthuysen (FW) transformation technique is used to reduce the Dirac Hamiltonian to a form suitable for direct interpretation in terms of the nonrelativistic part and a series of relativistic corrections. Derbenev and Kondratenko (DK) [17] used the FW technique to get their Hamiltonian for radiation calculations. Heinemann and Barber [18] have reviewed the derivation of the DK Hamiltonian and have used it to suggest a quantum formulation of Dirac particle beam physics, particularly for polarized beams, in terms of machine coordinates, observables, and the Wigner function.

In an independent and different approach an FW-like technique has been used to develop a systematic formalism of Dirac particle beam optics in which the aim has been to expand the Dirac Hamiltonian as a series of paraxial and nonparaxial approximations [8, 9, 10, 19, 20]. This leads to the reduction of the original 4-component Dirac spinor to an effective 2-component  $\psi(\underline{r}_\perp; z)$  which satisfies the accelerator optical Schrödinger equation [20]

$$i\hbar \frac{\partial}{\partial z} \psi(\underline{r}_\perp; z) = \hat{\mathcal{H}} \psi(\underline{r}_\perp; z) , \quad \psi(\underline{r}_\perp; z) = \begin{pmatrix} \psi_1(\underline{r}_\perp; z) \\ \psi_2(\underline{r}_\perp; z) \end{pmatrix} , \quad (22)$$

where  $\hat{\mathcal{H}}$  is a  $2 \times 2$  matrix operator incorporating the Stern-Gerlach (SG) spin-orbit effect and the Thomas-Bargmann-Michel-Telegdi (TBMT) spin evolution. As is usual in accelerator theory the spin operator  $\underline{S} = \frac{1}{2}\hbar \underline{\sigma}$  entering the accelerator optical Hamiltonian  $\hat{\mathcal{H}}$  refers to the rest frame of the moving particle. Further,  $(\hat{x}, \hat{y})$  and  $(\hat{p}_x, \hat{p}_y)$  in  $\hat{\mathcal{H}}$  correspond to the observed particle position and momentum components in the transverse plane. It should be noted that the 2-component  $\psi(\underline{r}_\perp; z)$  of Eq. (22) is an accelerator optical approximation of the original 4-component Dirac spinor, valid for any value of the design momentum  $p_0$  from nonrelativistic to extreme relativistic region.

For the normal magnetic quadrupole lens the accelerator optical Hamiltonian reads

$$\begin{aligned} \hat{\mathcal{H}} \approx & \frac{1}{2p_0} (\hat{p}_x^2 + \hat{p}_y^2) - \frac{1}{2}qK (\hat{x}^2 - \hat{y}^2) + \frac{1}{8p_0^3} (\hat{p}_x^2 + \hat{p}_y^2)^2 + \frac{q^2 K^2 \hbar^2}{8p_0^3} (\hat{x}^2 + \hat{y}^2) \\ & + \frac{(q + \gamma\epsilon)K}{p_0} (\hat{x}S_y + \hat{y}S_x) , \end{aligned} \quad (23)$$

where  $\gamma = E/mc^2$  and  $\epsilon = 2m\mu_a/\hbar$ . The last spin-dependent term accounts for the SG kicks in the transverse phase-space and the TBMT spin evolution. As in the Klein-Gordon case of Eq. (18),  $\hat{\mathcal{H}}$  of Eq. (23) also contains all the terms derivable from the classical theory plus the quantum correction terms. But, it must be noted that the scalar quantum correction term in Eq. (23) (4th term) is not the same as the 4th term in Eq. (18). Thus, besides in the  $\hbar$ -dependent effects of spin on the orbital quantum map (*e.g.*, the last term in Eq. (23)), even in the  $\hbar$ -dependent scalar quantum corrections the Dirac particle has its own signature different from that of the Klein-Gordon particle.

## 5 Conclusion

The problem of obtaining the quantum maps for phase-space transfer across particle beam optical systems has been reviewed. The leading quantum corrections to the classical maps are mainly due to the initial uncertainties and involve the Planck constant  $\hbar$  not explicitly but only through the minimum limits set by the uncertainty principle. These corrections can be obtained by direct quantization of the Lie algebraic formalism of classical particle beam optics. The Klein-Gordon and Dirac theories add further subtle,  $\hbar$ -dependent, corrections which may become effective when there are large fluctuations in the initial uncertainties. Contrary to the common expectation the scalar approximation of the Dirac theory is not completely equivalent to the Klein-Gordon theory. All aspects of quantum maps for spin- $\frac{1}{2}$  particle beams, including spin evolution and spin-orbit effects, can be studied, at the level of single particle dynamics, using the proper formalism based on the Dirac equation.

## Acknowledgements

I am grateful to M. Pusterla and R. Fedele who made it possible for me to participate in the QABP2K Workshop through financial support, by INFN-Napoli and INFN-Padova, for international travel, and accommodation expenses at Napoli and Capri. My special thanks are due to R. Fedele for the kind hospitality and stimulating



discussions during my visit to the INFN-Napoli. I am thankful to S. De Siena, S. De Martino, and F. Illuminati for the warm hospitality and useful discussions during my visit to the Department of Physics, University of Salerno, during the week of the Mini Workshop on Quantum Methodologies in Beam Physics.

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